

Parameter Estimation via Risk-Based Optimization

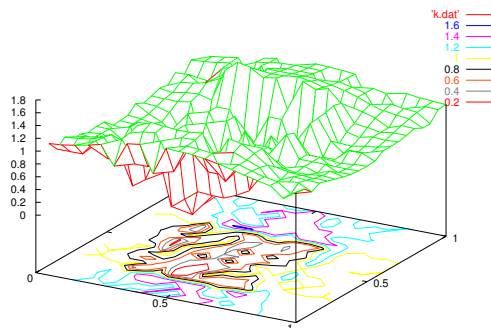
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Predictability of complex phenomena in physical systems with uncertain (under-determined by data) parameters is of central importance for many LANL programs. In practical applications, system parameters are often sampled at selected locations and their values elsewhere on the numerical grid are inferred through interpolation techniques, such as Kriging. This results in parameter distributions that are often much smoother than is realistic. We aim to replace the currently used interpolation techniques with an approach that uses risk-based optimization to populate the parameter space. Unlike traditional approaches that estimate parameter distributions without regard for critical behavior of a system, our parameter estimation approach can yield parameter distributions that correspond to system failure.

Several alternative approaches are used to assign the system parameter values to points of the computational domain where their measurements are not available. These can be grouped into two large groups: deterministic and probabilistic. Deterministic approaches, such as homogenization and upscaling, ascribe effective (homogenized) system parameters to the grid blocks of numerical models on the basis of smaller-scale random (or nonrandom) parameter values. This postulates local relationships between the relevant system states that are in fact nonlocal [1]. Among the probabilistic approaches, is the statistical technique referred to as Kriging [2]. Using linear or nonlinear interpolation schemes, a parameter field is constructed that fits best the statistics derived from an available data set. This method results in predicted system states that tend to be much smoother than their true counterparts.

We are developing a new paradigm for parameter estimation, which relies on risk-based op-

timization. Existing parameter estimation techniques result in predictions of system states that often miss system failures. Instead, in our approach, searching for system failures drives parameter estimation and determines their realizability.



Diffusion coefficient calculated via minimization with the objective to minimize the flux inside $(1/4, 3/4)^2$, a given average and variance, while its value at 30% of the grid points is fixed (sample points).

To demonstrate this, consider as a simple example the steady state diffusion equation on the unit square, where the diffusion coefficient D , a function of location, is given at a small number of sample points in the domain. We are interested in finding such D that satisfies some constraints, e.g. a given average \bar{D} and variance σ^2 . These parameters are determined by sample statistics. We investigate the set of all possible D by minimizing an objective function $G(D)$, to find best and worst case representatives

$$D = \arg \min_{D \in C} G(D). \quad (1)$$

Defining no-flow boundary conditions at the top and the bottom, and Dirichlet boundary conditions $u = 2$ on the left and $u = 1$ on the right hand boundary of the domain, we set

$$G(D) = w_1 \int_{(1/4, 3/4)^2} (D \nabla u)^2 dx dy + w_2 (\bar{D} - 1)^2 + w_3 (\sigma^2 - 0.1)^2,$$

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with weights w_i . The diffusion coefficient D that solves the minimization problem (1) results in the minimum flux $-D\nabla\mathbf{u}$ inside the region $(1/4, 3/4)^2$.

The figure shows the minimizer D_{min} on a 20×20 mesh. Here, we impose the constraint that 30% of the values of D (distributed uniformly on the computational grid) are set to one. The sample statistics are $\bar{D}_{min} = 0.999$, and $\sigma_{\bar{D}_{min}}^2 = 0$. The coefficient D is clearly lowest inside the area $(1/4, 3/4)^2$, while still satisfying all imposed constraints. An interpolation based approach, such as Kriging, would result in a much smoother coefficient D . If a system failure was thought to be associated with a very low value of D , then using our approach it is possible to assess the likelihood of such an occurrence.

More complex examples will require better optimization algorithms. Such examples can easily generate very large optimization problems. We aim to develop new and improve existing optimization algorithms to make our new approach to parameter estimation practical.

In conclusion, risk-based parameter estimation paired with efficient optimization techniques is precisely what is needed to increase confidence in predictions that are based on limited parameter data.

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References

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